

1 Coordination chemistry of Co complexes containing tridentate SNS ligands and their application as
2 catalysts for the oxidation of n-octane

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5 Table S1: Crystallographic data collection and refinement parameters

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Empirical formula	C ₁₈ H ₂₆ Cl ₄ Co ₂ N ₂ S ₄	C ₁₁ H ₁₇ Cl ₂ CoNS ₂	C ₁₅ H ₂₅ Cl ₂ CoNS ₂	C ₁₉ H ₁₇ C ₁₂ CoNS ₂
Formula weight	658.31	357.21	413.31	453.29
Wavelength/Å	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P-1	Cc	C2/c	P21/c
<i>a</i> /Å	7.5980(2)	24.9529(9)	34.5930(9)	10.6720(5)
<i>b</i> /Å	8.4802(2)	7.9877(3)	7.6101(2)	8.4107(4)
<i>c</i> /Å	10.5727(3)	16.5411(6)	15.5012(4)	23.5413(11)
<i>α</i> /°	80.6050(10)	90	90	90
<i>β</i> /°	83.4030(10)	112.111(2)	99.7340(10)	114.791(2)
<i>γ</i> /°	69.8060(10)	90	90	90
<i>V</i> /Å ³	629.51(3)	3054.44(19)	4022.04(18)	1918.31(16)
<i>T</i> /K	173(2)	173(2)	173(2)	173(2)
<i>Z</i>	1	8	8	4
<i>D_c</i> /Mg m ⁻³	1.736	1.554	1.365	1.570
<i>μ</i> /mm ⁻¹	2.085	1.725	1.320	1.393
<i>F</i> (000)	334	1464	1720	924
Reflections collected	10432	13589	16675	54122
Crystal size/mm ³	0.53 x 0.27 x 0.21	0.15 x 0.10 x 0.04	0.434 x 0.371 x 0.20	0.38 x 0.13 x 0.13
<i>θ</i> /range/°	1.96-28.00	1.76-27.00	2.39-26.00	1.91-28.00
Index ranges	-8 ≤ <i>h</i> ≤ 10, -11 ≤ <i>k</i> ≤ 11, -13 ≤ <i>l</i> ≤ 13	-31 ≤ <i>h</i> ≤ 31, -10 ≤ <i>k</i> ≤ 10, -21 ≤ <i>l</i> ≤ 21	-42 ≤ <i>h</i> ≤ 40, -9 ≤ <i>k</i> ≤ 9, -18 ≤ <i>l</i> ≤ 18	-14 ≤ <i>h</i> ≤ 14, -11 ≤ <i>k</i> ≤ 11, -31 ≤ <i>l</i> ≤ 31
Independent reflections, <i>R_{int}</i>	3035, 0.0390	6536, 0.0597	3959, 0.0368	4594, 0.0271
Max., min. transmission	0.6686, 0.4046	0.9364, 0.8378	0.7913, 0.6118	0.8397, 0.6197
Data, restraints, parameters	3035, 0, 138	6536, 2, 311	3959, 48, 168	4594, 0, 227
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.0310, 0.0773	0.0551, 0.1268	0.0679, 0.2236	0.0695, 0.1865
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0366, 0.0797	0.0850, 0.1756	0.0829, 0.2428	0.0719, 0.1876
Goodness-of-fit on <i>F</i> ²	1.124	1.039	1.079	1.161
CCDC number	984366	984367	984368	984369

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